This report is approved for public release.

Final Report

1. Grant Title: "Computational Study of Correlated Electrons"

2. Principal Investigator: Prof. Elbio Dagotto (Florida State University). Co-PI's: Prof. Adriana Moreo (Florida State University) and Prof. Richard T. Scalettar (Univ. of California at Davis).

3. Grant Number: ONR-N00014-93-1-0495

4. Funding Profile: the total grant amount was $305,212. Grant period: 6/1/93 to 28/2/96.

5. Technical Objectives:

- Study the phase diagram of models of strongly correlated electrons for the high temperature superconductors.
- Study the development of magnetism as a function of band filling, temperature, and ratio of correlation energy to bandwidth, in tight binding models.
- Compare theoretical predictions for angle-resolved photoemission with existing experimental data.

6. Published papers resulting from this support:

   a. Submitted but not published: 05
   b. Published in refereed journals: 43
   c. Published in non-refereed journals: 00

7. Number of technical reports submitted: 0

8. Number of books written: 0

9. Number of book chapters written: 3

10. Patents as a result of this work.

a. Number of applications filed: 0
b. Number of patents granted: 0

11. Total number of presentations given: 78

- Richard Scalettar: "Magnetic Properties of Coupled Hubbard Planes", invited talk, *International Euroconference on Magnetic Correlations*, Würzburg, Germany, September 1994. The phase diagram of the Hubbard model on bilayer systems was established numerically.
- Adriana Moreo: "Study of ARPES data and d-wave superconductivity: a progress report", invited talk, Conference on *Spectroscopies in Novel Superconductors*, Stanford University, Stanford, USA, March 1995. Part of the angle-resolved photoemission data for the cuprates was explained using simple models for the cuprates.
- Elbio Dagotto: "Flat quasiparticle dispersion in the t-J model", invited talk, March meeting of the APS, San Jose, USA, March 1995. Recently experimentally observed flat bands in the cuprates are described as caused by antiferromagnetic correlations in the t-J model.

12. Honors and awards received during the granting period:

- Dagotto: Developing Scholar Award, Florida State University, April 1995, $6,000 to conduct research.
- Ulmk e: Research Grant of the Deutsche Forschungsgemeinschaft (DFG) for research on the topic "Magnetism and Metal-Insulator Transitions in Disordered, Interacting Electron Systems", from 4/1/95 until 5/31/96, total: DM28,000, approx. $18,000. (Dr. M. Ulmke is a postdoc supported by the grant ONR-N00014-93-1-0495).

13. Number of different post-docs supported at least 25% of the time for at least one calendar year: 3. Total person-months of post-doc supported under this grant: 40.

14. Number of different graduate students supported at least 25% of the time for at least one calendar year: 1. Total person-months of graduate student support under this grant: 15.

15. Most significant publications resulting from this work:

- "Antiferromagnetic and van Hove scenarios for the cuprates: Taking the best of both worlds", E. Dagotto, A. Nazarenko and A. Moreo, Phys. Rev. Lett. **74**, 310 (1995). A theory for the cuprates is discussed. Ingredients of previous theories that used antiferromagnetic correlations and van Hove effects are mixed in a single scenario.
- "Magnetic and Pairing Correlations in Coupled Hubbard Planes", R.T. Scalettar, J.W. Cannon, D.J. Scalapino, and R.L. Sugar, Phys. Rev. **B50**, 13419 (1994). This paper examined the competition between antiferromagnetism and singlet formation in a

model of layered magnets. It was found that above a certain critical amount of electron hopping between the layers, magnetic order is destroyed.

- " Antiferromagnetically Induced Photoemission Band in the Cuprates", S. Haas, A. Moreo, and E. Dagotto, Phys. Rev. Lett. **74**, 4281 (1995). A numerical study of antiferromagnetic induced bands in the cuprates is reported. A comparison with photoemission experiments is made.

- "Magnetic Phase Diagram of the Hubbard Model", J. K. Freericks and Mark Jarrell, Phys. Rev. Lett. **74**, 186 (1994). This paper was the first computation of the magnetic phase diagram of a widely used model of interacting electrons. The dependence of the transition temperature to a magnetic state on the electron density and interaction strength was determined. (Dr. J. Freericks is a postdoc supported by the grant ONR-N00014-93-1-0495).

- "Correlated Electrons in High Temperature Superconductors", E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994). An extensive review of high temperature superconductors is provided. Over 500 references are given. The emphasis is on the comparison between theory and experiments.

16. Major accomplishments:

- Phase diagrams of models of magnetism and superconductivity were determined using classical and quantum Monte Carlo methods, exact diagonalization techniques, and analytic approximations. Among the models studied are the one and three band Hubbard models, the t-J model, and their many variations and generalizations.
- A theory for the cuprates was proposed based on the behavior of holes near a half-filled band. Several predictions for experiments were made.
- An extensive comparison of available experimental angle-resolved photoemission data and theoretical predictions was made. Excellent agreement was observed in a variety of high-Tc compounds. Flat and shadow bands in the cuprates were found in numerical studies of the t-J and Hubbard models.
- The nature of the superconducting-insulator phase transition in 2-d disordered superconductors was determined.
- New techniques to simulate interacting electron systems, including Quantum Monte Carlo, Strong Coupling Expansions, and Conserving Approximations were developed.
- The presence of superconductivity near phase separation in several models of high-Tc cuprates was established.

17. Transitions: None

18. Summary of the overall impact of the research:

We applied quantum simulation techniques to a number of the most outstanding problems in the physics of solids, with a particular emphasis on magnetism and superconductivity. We also further developed these techniques in significant new directions. Several experimental results have been explained by our theoretical calculations and

simulations. New theories for the high-temperature superconductors have been proposed. Metamagnetic transitions and ferromagnetism have been analyzed. A new area of research (ladder systems) has been developed.

The original objectives of the proposal have been accomplished. A vast amount of additional information on models of correlated electrons has been documented. New directions of research have been identified.

19. Key words describing the project:

    High-Tc Superconductors, Quantum Simulations, Magnetism, D-wave Pairing.

20. Viewgraphs: one set enclosed.

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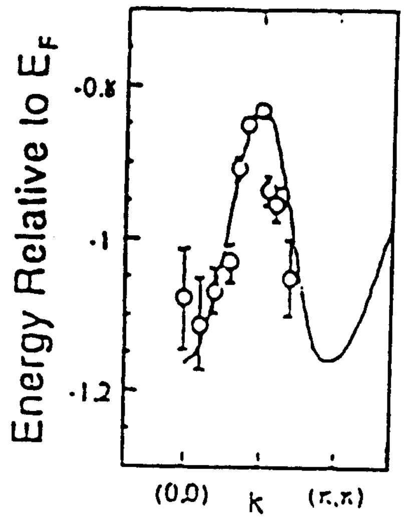
Scientific Highlights

- Photoemission data in cuprate materials in agreement with theoretical results.



- Our AFVH model predicts T_c vs $< n >$ in agreement with experiments.